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NUMERICAL INTEGRATION OF FLOW IN A ROTATING ANNULUS III: SOLUTION OF POISSON'S EQUATION

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Definition of symbols.

General:	x, y, z	spatial co-ordinates	
	t	time co-ordinate	
	Π	pressure field	
In §2:	g	acceleration due to gravity	
	$\underset{\sim}{u}$	velocity vector field	
	u, v, w	components of velocity vector	
	$\underset{\sim}{S}$	velocity source function vector field	
	S_u, S_v, S_v	components of source function vector	
	ρ	density	
	Ξ	a modified pressure field	
In §3 to §7:	c_{ij}	coupling constants	Eqn. 3.8
	S	the divergence of $\underset{\sim}{S}$ above	
	u_i	eigenvectors of $\partial^2/\partial x^2$ operator	Eqn. 3.7
	v_i	orthogonal combinations of u_i	Eqn. 4.3
	$\delta x_i, \delta\tilde{x}_i$;	grid intervals	Fig. 2
	δ_{ij}	Kronecker delta [= 1 if i = j, = 0 otherwise]	
	$\epsilon_{ik}, \gamma_{ik}$	expansion coefficients	Eqn. 3.5
	Δ_i	a determinant of order i	
	λ_i	eigenvalues of $\partial^2/\partial x^2$ operator	Eqn. 3.7
	σ_{ik}, β_{ik}	overlap integrals	Eqns. 3.6, 4.4
	$\mathbb{1}$	a unit matrix [ijth element = δ_{ij}]	

1. INTRODUCTION

The most time-consuming operation in the numerical solution of the Navier-Stokes equations (described previously by Farnell and Plumb, 1975 and 1976, hereafter referred to as FP I and FP II respectively) is the solution of the Poisson equation to yield the pressure field. The most efficient method of solution is used by Williams (1969) and involves reduction of the original equation to many one-dimensional equations (which may be solved by Gaussian elimination) by means of Fourier Transforms; the Fourier Transforms can be made relatively fast (Cooley and Tukey, 1965) for cases where the number of points can be factorised into small integers. However the technique is not applicable in problems where the variables are represented on non-uniformly spaced grid-points, as is desirable when thin boundary layers are to be resolved, since trigonometric functions are not orthogonal on such a mesh. (A list of properties of discrete Fourier Transforms is given by Gentleman and Sande, 1966). Thus it was necessary to use an iterative method in the original formulation of the numerical models (FP I §5.1), viz the ADI method of Peaceman and Rachford (1955) as optimised by Wachspress (1966) (see also Varga, 1962). This leads to errors which may be interpreted as non-zero divergence of the velocity vector, which lead to inaccuracies in the conservation of integral properties such as angular momentum (FP I §4.4).

This report describes a direct method of solution of Poisson's equation on a non-uniform grid, which is an extension of the Fourier transform technique and reduces to that technique in special cases. This method has the following properties:

(i) An analogue of the usual discrete Fourier transform is performed using orthogonal functions peculiar to the mesh being employed; the functions are not unique except in special circumstances which will be given in §5; one such case is the usual Fourier transform on a uniform mesh.

(ii) Since the points are non-uniform, the magnitude of one of the functions at a given point will not be identical to its magnitude at any other point, so that fast transforms are precluded. However if any symmetry is present e.g. the grid points on one side of the centre are reflections of those on the

other side (this is the usual case for annulus models), then advantage may be taken of this to generate a "slightly fast" transform. Even so, for large numbers of gridpoints (larger than those actually employed) the ADI iterative method is more favourable computationally (see § 7).

(iii) The method may be readily adapted to Neumann, Dirichlet and periodic boundary conditions.

(iv) The accuracy of the results is limited only by the rounding error in computation. There is no need for an initial guess.

2. FORMULATION OF POISSON'S EQUATION

2.1 Basic derivation

The momentum equations may be written in the following form (cf. FP I § 4.5.

$$\frac{\partial \underset{\sim}{u}}{\partial t} = -\nabla \Pi + \underset{\sim}{S} \tag{2.1}$$

Taking the divergence of this equation yields

$$\frac{\partial \nabla.\underset{\sim}{u}}{\partial t} = -\nabla^2 \Pi + \nabla.\underset{\sim}{S} \tag{2.2}$$

which by virtue of the continuity equation

$$\nabla.\underset{\sim}{u} = 0 \tag{2.3}$$

becomes

$$\nabla^2 \Pi = \nabla.\underset{\sim}{S} \tag{2.4}$$

which is the Poisson equation. The boundary conditions appropriate to annulus integrations are that all variables shall be periodic in the azimuthal direction, and that

$$\frac{\partial u}{\partial t} = -\frac{\partial \Pi}{\partial r} + S_u \tag{2.5}$$

at the sidewalls and

$$\frac{\partial w}{\partial t} = -\frac{\partial \Pi}{\partial z} + S_w \tag{2.6}$$

at the endwalls. For many purposes the boundary conditions on velocity are such that equations (2.5) and (2.6) may be simplified to the following.

$$\frac{\partial \pi}{\partial r} = S_u \quad ; \quad \frac{\partial \pi}{\partial z} = S_w \tag{2.7}$$

2.2 Modification of the boundary conditions

It has been noted (FP I §4.5) that the boundary conditions may be further simplified by substituting

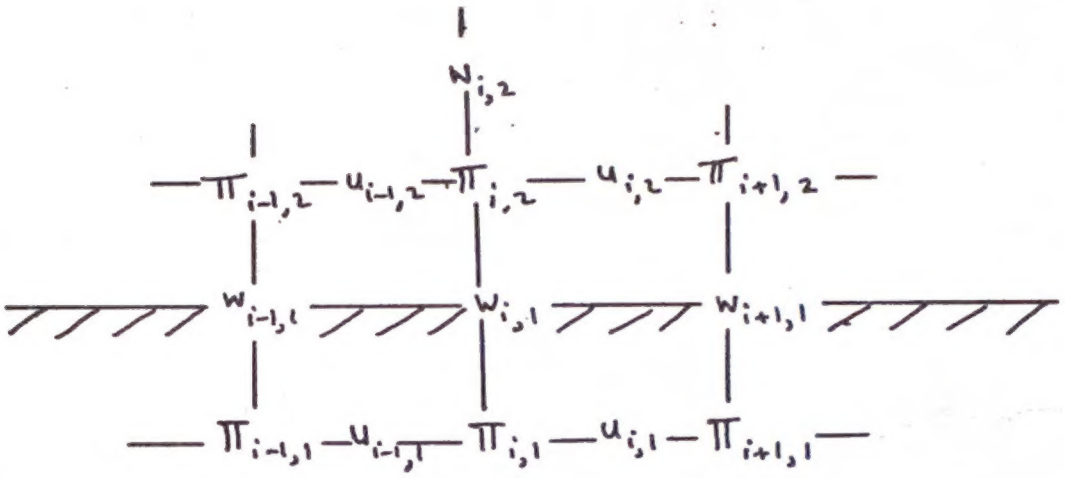
$$\frac{\partial \pi}{\partial r} = 0 \quad ; \quad \frac{\partial \pi}{\partial z} = 0 \tag{2.8}$$

for equations (2.7) (G O Roberts, private communication). This is further considered here.

First, note that the boundary condition to be applied to the normal component of velocity (e.g. w_i, in Figure 1, which is adapted from FP I figure 1) must be consistent with the velocity fields produced by the momentum equations (2.1), else the continuity equation (2.3) will not be satisfied at the point corresponding to π_{i2}. Since these fields derive in part from application of the boundary conditions at the previous timestep, the boundary conditions must be consistent not only in space but also in time. Within this limitation, it is not necessary to determine the pressure gradient $\frac{\partial \pi}{\partial z}$ at the w_{i1} point since it will never be used: the velocity is set by the boundary condition which is applied. Since the normal finite-difference equations are not applicable at this point, it is a great advantage not to have to evaluate a source function here, which evaluation would have to be performed by means of a Taylor series expansion (Pearson, 1965). In fact it is enough to let the normal component of the source function vanish at all points on boundaries, which converts equation (2.7) to (2.8). This also means that $\nabla . \underset{\sim}{S}$ in equation (2.4) has been altered, but this precisely cancels the effect of the modified boundary conditions. (Note that a set of boundary conditions obtained from the components of a vector field, of which the divergence is used to generate the pressure source, is necessarily consistent.)

Figure 1

Arrangement of variables at lower boundary.



It is not possible to set the source function to be zero and also use a zero-gradient boundary condition if the boundary normal velocity is time dependent, since the term corresponding to $\frac{\partial \nabla . \underset{\sim}{u}}{\partial t}$ in equation (2.2) does not then vanish. If the zero-gradient conditions (2.8) are retained then the source function must be defined by equation (2.9) at the boundary points.

$$S_u = \frac{\partial u}{\partial t} \quad ; \quad S_w = \frac{\partial w}{\partial t} \tag{2.9}$$

To illustrate the above remarks consider the two-dimensional problem defined by equations (2.10).

$$\frac{\partial u}{\partial t} + \frac{\partial \Pi}{\partial x} = S_u \quad ; \quad \frac{\partial w}{\partial t} + \frac{\partial \Pi}{\partial z} = S_w \tag{2.10}$$

$$\frac{\partial^2 \Pi}{\partial x^2} + \frac{\partial^2 \Pi}{\partial y^2} = \frac{\partial S_u}{\partial x} + \frac{\partial S_w}{\partial z}$$

The relevant conditions at the boundary (x = 0) are

$$\frac{\partial u}{\partial t} = 0 \quad ; \quad \frac{\partial \Pi}{\partial x} = S_u = g \, . \tag{2.11}$$

The solution Π is determined only insofar as an arbitrary constant may be added to the field. Now take another Poisson equation

$$\frac{\partial^2 \tilde{\tilde{\Xi}}}{\partial x^2} + \frac{\partial^2 \tilde{\tilde{\Xi}}}{\partial z^2} = \frac{\partial S_u}{\partial x} + \frac{\partial S_w}{\partial z} - \frac{\partial \alpha}{\partial x} \qquad (2.12)$$

where α is a function which is zero everywhere except for an infinitesimal region at x = 0 where $\alpha = -\rho$. Clearly $\tilde{\tilde{\Xi}}$ is a solution to these equations, excepting the x = 0 region, if it is identical to Π. At the boundary

$$\frac{\partial^2 \tilde{\tilde{\Xi}}}{\partial x^2} + \frac{\partial^2 \tilde{\tilde{\Xi}}}{\partial z^2} = \frac{\partial \rho}{\partial x} + \frac{\partial S_w}{\partial z} - \frac{\partial \rho}{\partial x} = \frac{\partial S_w}{\partial z} \qquad (2.13)$$

and so

$$\frac{\partial^2 \Pi}{\partial x^2} + \frac{\partial^2 \Pi}{\partial z^2} = \frac{\partial \rho}{\partial x} + \frac{\partial S_w}{\partial z} = \frac{\partial^2 \tilde{\tilde{\Xi}}}{\partial x^2} + \frac{\partial^2 \tilde{\tilde{\Xi}}}{\partial z^2} + \frac{\partial \rho}{\partial x} \qquad (2.14)$$

of which a solution is

$$\frac{\partial \tilde{\tilde{\Xi}}}{\partial x} = \frac{\partial \Pi}{\partial x} - \rho = 0 \qquad (2.15)$$

which is the boundary condition which was to be imposed. Thus the only change to the solution if the procedure outlined is performed is to the normal gradient on the boundary, and as indicated above this is irrelevant.

2.3 Modification of the source function

From the definition of S_w (see the momentum equations, FP I equation 2.3) it is apparent that since density is formulated as

$$\rho = \rho_0 + \rho'(T) \qquad (2.15)$$

then the pressure Π may be written as

$$\Pi = \Pi_0 + \Pi' \qquad (2.16)$$

where Π_0 is chosen such that

$$\frac{\partial \Pi_0}{\partial z} = g. \qquad (2.17)$$

Then the buoyancy term may be written as $g\,\rho'/\rho_0$ and Π' used within the integration. This means that the pressure variable is reduced by $\sim 10^3$ in magnitude while its range of variation is the same, an important gain for preserving precision. It nevertheless still requires the Poisson solution to be performed in double precision ($\sim$ 16 decimals). A further improvement is made if the buoyancy term is modified further, as

$$\rho'' = \rho' - \bar{\rho}(z) \tag{2.18}$$

where the horizontal mean is removed (P J Mason, private communication).

It is easy to see that in fact the mean of each component of the source function (averaged over the two other co-ordinates) may be subtracted without affecting the final result. For let

$$\underset{\sim}{S} = \underset{\sim}{\alpha} + (0, 0, \beta(z)) \tag{2.19}$$

so that

$$\nabla . \underset{\sim}{S} = \nabla . \underset{\sim}{\alpha} + \frac{\partial \beta}{\partial z} \tag{2.20}$$

If the equation

$$\nabla . \underset{\sim}{\alpha} = \nabla^2 \underset{\sim}{\Xi} \tag{2.21}$$

is solved for $\underset{\sim}{\Xi}$, then

$$\nabla^2 \Pi = \nabla . \underset{\sim}{S} = \nabla^2 \underset{\sim}{\Xi} + \frac{\partial \beta}{\partial z} \tag{2.22}$$

which is satisfied by

$$\Pi = \Xi + \int \beta \, dz \, . \tag{2.23}$$

Substitution into equation (2.1) yields

$$\frac{\partial \underset{\sim}{u}}{\partial t} = -\nabla \underset{\sim}{\Xi} + \underset{\sim}{\alpha} \tag{2.24}$$

which is the desired result.

3. THEORY OF THE DIRECT SOLUTION OF POISSON'S EQUATION

The analysis will be given for a two-dimensional mesh which is rectilinear in Cartesian co-ordinates; it is readily extendable to higher dimensions and other co-ordinate systems. Under these circumstances equation (2.4) is rewritten as

$$\frac{\partial^2 \pi}{\partial x^2} + \frac{\partial^2 \pi}{\partial y^2} = S(x,y) \tag{3.1}$$

where the notation for the source function has been changed.

The method entails expressing the variables π and S as an expansion in functions V_i which are a function of one co-ordinate (say x) only.

$$\pi = \sum_i P_i(y)\, V_i(x) \quad ; \quad S = \sum_i Q_i(y)\, V_i(x) \tag{3.2}$$

The functions will be chosen so that they are orthogonal and normalised:

$$\int V_i V_j = \delta_{ij} \tag{3.3}$$

where the limits of integration depend on the domain of interest. For an analytic solution the series is necessarily infinite, but the series is obviously truncated in the numerical case according to the number of grid points.

It is possible to generate as many equations as these are functions V_i by multiplying equation (3.1) by each in turn and integrating over x.

$$V_j \frac{\partial^2}{\partial x^2}\left(\sum_i P_i V_i\right) + V_j \frac{\partial^2}{\partial y^2}\left(\sum_i P_i V_i\right) = V_j \sum_i Q_j V_j$$

$$\Rightarrow V_j \sum_i P_i \frac{\partial^2 V_i}{\partial x^2} + V_j V_i \frac{\partial^2 P_i}{\partial y^2} = \sum_i Q_i V_i V_j$$

$$\Rightarrow \sum_i P_i \int V_j \frac{\partial^2 V_i}{\partial x^2}\, dx + \frac{\partial^2 P_j}{\partial y^2} = Q_j \tag{3.4}$$

Note that equation (3.3) has been used.

It is convenient to evaluate the integral in equation (3.4) by expanding the functions V_i in terms of functions u_k which are eigenfunctions of the $\frac{\partial^2}{\partial x^2}$ operator.

$$V_i = \sum_k \gamma_{ik} u_k \quad ; \quad u_k = \sum \epsilon_{ki} V_i \tag{3.5}$$

For a complete expansion the sets of functions v_i and u_k must contain the same number of members. The functions u_k are assumed to be normalised but are not necessarily orthogonal.

$$\int u_i u_k \, dx = \sigma_{ik} \qquad (3.6)$$
$$= 1 \quad \text{if} \quad i=k$$

The eigenvalues will be denoted by λ_k, defined as follows.

$$\frac{\partial^2}{\partial x^2}(u_k) = \lambda_k u_k \qquad (3.7)$$

(In analytic theory the eigenfunctions are trigonometric functions $\sin(mx)$ and $\cos(mx)$ with eigenvalues $-m^2$.)

The equations (3.5) are substituted into the integral in equation (3.4) as follows.

$$\int v_j \frac{\partial^2 v_i}{\partial x^2} dx = \int v_j \frac{\partial^2}{\partial x^2}\left(\sum_k \gamma_{ik} u_k\right) dx$$

$$= \int v_j \sum_k \gamma_{ik} \frac{\partial^2 u_k}{\partial x^2} dx$$

(using 3.7)
$$= \int v_j \sum_k \gamma_{ik} \lambda_k u_k \, dx$$

$$= \int v_j \sum_k \gamma_{ik} \lambda_k \left(\sum_l \epsilon_{kl} v_l\right) dx$$

$$= \int v_j \sum_l v_l \left\{\sum_k \gamma_{ik} \lambda_k \epsilon_{kl}\right\} dx$$

(using 3.3)
$$= \sum_k \gamma_{ik} \lambda_k \epsilon_{kj} \equiv c_{ij} \qquad (3.8)$$

This serves to define the "coupling constants" c_{ij} which connect the following set of equations, derived from equations (3.4), together.

$$\sum_i c_{ij} P_i + \frac{\partial^2 P_j}{\partial y^2} = Q_j \qquad (3.9)$$

It would be possible to solve equation (3.9) if all of the constants c_{ij} were zero apart from c_{jj}; this is the principle of the standard technique on a uniform grid. In the general case it is possible to choose the constants such that they obey the following relationship:

$$c_{ij} = 0 \quad \text{if} \quad j > i \qquad (3.10)$$

and this is described in section 4. Assuming (3.10), equation (3.9) becomes

$$\frac{\partial^2 P_j}{\partial y^2} + c_{jj} P_j = Q_j - \sum_{i>j} c_{ij} P_i \qquad (3.11)$$

which may be solved when j has its maximum values; the result is substituted into all other equations, effectively as a correction to Q_j, and the next lower equation can now be solved. Thus all of the P_j are determined, in reverse order, and may be substituted into equation (3.2) to generate the required Π field.

4. GENERATION OF ORTHOGONAL FUNCTIONS

Given a set of functions u_k defined by equation (3.7), a set of orthogonal functions may be obtained using the Schmidt procedure (Wilkinson, 1965). The first function v_1 may be chosen as identical to u_1. The second function must be chosen as a linear combination of u_1 and u_2 such that the conditions (3.3) are met.

Let $v_2 = A(u_2 + \alpha v_1) = A(u_2 + \alpha u_1)$: Then

$$\int v_1 v_2 \, dx = \int u_1 A(u_2 + \alpha_2 u_1) \, dx = A\sigma_{12} + A\alpha = 0 \qquad (4.1)$$

using (3.6) and (3.3). Thus $\alpha = -\sigma_{12}$, and

$$\int v_2^2 \, dx = A^2 \int u_2^2 + \alpha^2 u_1^2 + 2\alpha u_1 u_2 \, dx$$
$$= A^2 (1 - \sigma_{12}^2) = 1 \qquad (4.2)$$

so that A is determined. This procedure may be continued to generate the remaining v_i ; the general solution is:

$$v_i = \sqrt{\frac{1}{1 - \sum_{k<i} \beta_{ik}^2}} \left(u_i - \sum_{k<i} \beta_{ik} v_{ik} \right) \qquad (4.3)$$

where

$$\beta_{ik} = \int u_i v_k \, dx \qquad (4.4)$$

Equation (4.3) may be rearranged to give the constants ϵ_i of equation (3.5).

$$u_i = \sqrt{1 - \sum_{k<i} \beta_{ik}^2} \, v_i + \sum_{k<i} \beta_{ik} v_k$$

i.e.

$$\left.\begin{aligned} \epsilon_{ki} &= \beta_{ik} \qquad (\text{for } k<i) \\ \epsilon_{ii} &= \sqrt{1 - \sum_{k<i} \beta_{ik}^2} \\ \epsilon_{ki} &= 0 \qquad (\text{for } i>k) \end{aligned}\right\} \qquad (4.5)$$

It may also be seen that

$$\left.\begin{aligned} \gamma_{ii} &= \frac{1}{\epsilon_{ii}} \\ \gamma_{ik} &= 0 \qquad (\text{for } k \geq i) \\ \text{and} \quad \gamma_{ii} &= 1 \end{aligned}\right\} \tag{4.6}$$

where γ_{ik} are also defined in (3.5). The remaining constants may be determined recursively.

$$\begin{aligned} v_i &= \frac{u_i}{\epsilon_{ii}} - \sum_{k<i} \frac{\epsilon_{ki}}{\epsilon_{ii}} v_k \\ &= \frac{u_i}{\epsilon_{ii}} - \sum_{k<i} \frac{\epsilon_{ki}}{\epsilon_{ii}} \left\{ \sum_{l \leq k} \gamma_{kl} u_l \right\} \\ &= \frac{u_i}{\epsilon_{ii}} - \sum_{l<i} u_l \left\{ \sum_{k \geq l} \frac{\epsilon_{ki}}{\epsilon_{ii}} \gamma_{kl} \right\} \end{aligned}$$

i.e.

$$\gamma_{il} = -\sum_{k=l}^{i-1} \frac{\epsilon_{ki}}{\epsilon_{ii}} \gamma_{kl} \tag{4.7}$$

Using the definitions (4.5 - 4.7), equation (3.8) becomes

$$\begin{aligned} c_{ij} &= \sum_{k=j}^{i} \gamma_{ik} \lambda_k \epsilon_{kj} \qquad (\text{for } j \leq i) \\ &= 0 \qquad\qquad\qquad\quad (\text{for } j > i) \end{aligned} \tag{4.8}$$

so that relation (3.10) is satisfied.

5. NUMERICAL IMPLEMENTATION OF THE DIRECT POISSON EQUATION SOLUTION

The above analysis may be carried through, substituting vectors (with as many components as there are gridpoints) for the functions v_i and u_k, and replacing integrations by the scalar products of the vectors. The determination of u_k becomes a matrix eigenvalue problem. Using a three-point numerical operator, such as is incorporated in the models described in FP I and II, the problem is as follows. Figure 2 shows the arrangement of gridpoints, and is an adaptation of FP I figure 1. Equation (3.7) becomes

$$\frac{\dfrac{u_{i+1}-u_i}{\delta\tilde{x}_{i+1}} - \dfrac{u_i-u_{i-1}}{\delta\tilde{x}_i}}{\delta x_i} = \lambda u_i \tag{5.1}$$

To close the problem it is necessary to provide boundary conditions relating u_1 to u_2 and u_I to u_{I-1} where I is the number of points. These may be used to eliminate u_1 and u_I from (5.1), leaving a tridiagonal matrix of dimension $I-2$.

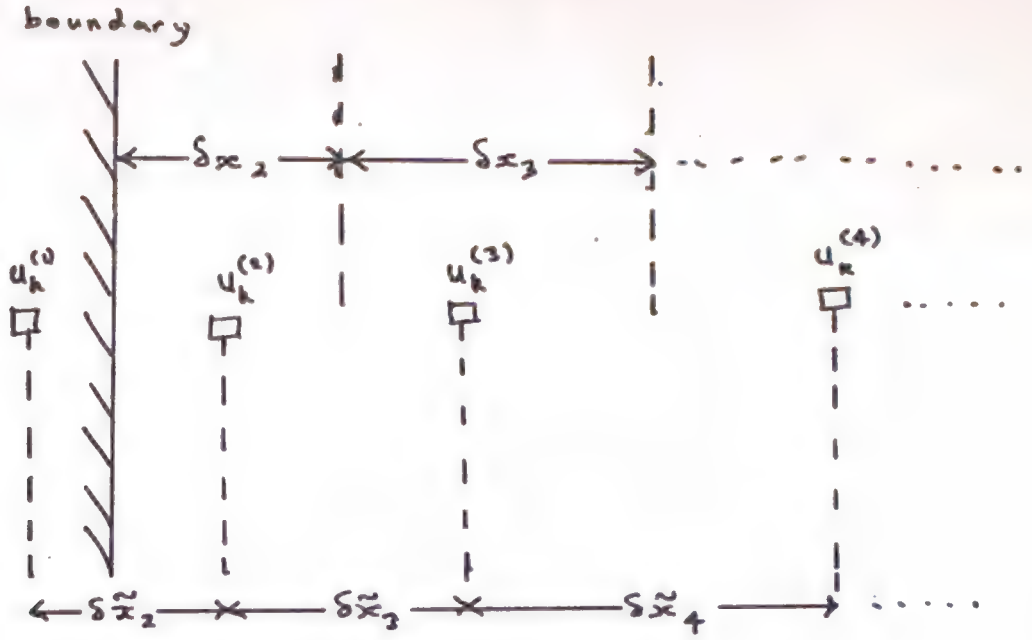


Figure 2 Distribution of gridpoints on which Π, S, u, v are defined, with definition of grid intervals.

$$\begin{pmatrix} \alpha_1 & \beta_2 & 0 & 0 & \\ \gamma_2 & \alpha_2 & \beta_3 & 0 & \\ 0 & \gamma_3 & \alpha_3 & \beta_4 & \\ \text{zeros} & & \ddots & \ddots & \ddots \end{pmatrix} \begin{pmatrix} u_2 \\ u_3 \\ u_4 \\ \vdots \end{pmatrix} = \lambda \begin{pmatrix} u_2 \\ u_3 \\ u_4 \\ \vdots \end{pmatrix} \qquad (5.2)$$

where $\beta_i = \dfrac{1}{\delta\tilde{x}_{i+1}\,\delta x_i}$; $\gamma_i = \dfrac{1}{\delta\tilde{x}_{i+1}\,\delta x_{i+1}}$; $\alpha_i = -\beta_{i+1} - \gamma_i$;

except that α_1 and α_{I-2} are modified by the boundary conditions to include γ_1 and β_{I-1} respectively. It may be observed that this matrix is quasi-symmetric, i.e. all elements are real, and $\beta_i \gamma_i > 0$ (Wilkinson, 1965), and it is therefore always possible to effect a similarity transform to a real symmetric tridiagonal matrix in which the diagonal elements are still α_i and the superdiagonal elements are $\sqrt{\beta_i \gamma_i}$. The eigenvalues of this new matrix may be determined by bisection: a bound to the absolute value of the eigenvalues is given by the maximal sum of elements in a row, and having thus obtained an upper and lower limit, the interval is bisected until the limits agree to within the required tolerance. As a

criterion of whether the mean of the old limits constitutes an upper or lower bound, the Sturm sequence property is employed. Consider the following determinants (which are the leading minors of the matrix).

$$\Delta_1 = |a_1| \;,\; \Delta_2 = \begin{vmatrix} a_1 & b_2 \\ b_2 & a_2 \end{vmatrix} \;,\; \Delta_3 = \begin{vmatrix} a_1 & b_2 & 0 \\ b_2 & a_2 & b_3 \\ 0 & b_3 & a_3 \end{vmatrix} \;, \ldots\ldots$$

where $a_i = \alpha_i - \lambda_g$ (λ_g is a guessed eigenvalue) and $b_i = \sqrt{\beta_i \gamma_i}$. These are arranged in order together with Δ_0 which is defined as unity. (This allows a simple recursion formula

$$\begin{aligned} \Delta_0 &= 1 \\ \Delta_1 &= a_1 \\ \Delta_i &= a_i \Delta_{i-1} - b_i^2 \Delta_{i-2} \end{aligned} \qquad (5.3)$$

to be used.) Within this series it is necessary to count the number of times that Δ_i and Δ_{i-1} are of the same sign, considering $\Delta_i = 0$ to have the opposite sign to Δ_{i-1}, and noting that successive zeros are impossible. The number thus obtained is identical to the number of eigenvalues which are greater than λ_g.

Thus all eigenvalues may be determined in turn. It may be noted that if $\gamma_i = \beta_{i+1}$ for all i, then the matrix of equation (5.2) is already symmetric, and therefore has orthogonal eigenvectors. In the cartesian problem this implies that all the grid intervals δx and $\delta \tilde{x}$ are equal, and this corresponds to the orthodox Fast Fourier Transform technique.

The eigenvectors may be determined by substituting each eigenvalue back into equation (5.2). Since the vectors may be multiplied by an arbitrary constant and still remain solutions, Gaussian elimination will yield an indeterminate result for the last step of the forward elimination; the constant is of course selected to ensure normalisation. Direct solution is liable to generate unbounded errors even for small matrices (Wilkinson, 1965), and the following iterative method may be used instead. Denote the matrix by $\underset{\approx}{A}$ and a guessed vector by $\underset{\sim}{b}_i$. Consider now the equation

$$\left(\underset{\approx}{A} - \lambda_g \mathbb{1}\right) \underset{\sim}{b}_{i+1} = \underset{\sim}{b}_i \qquad (5.4)$$

where λ_g is an approximation to the exact eigenvalue. Let

$$\underset{\sim}{b}_i = \sum_k \gamma_k^{(i)} u_k \tag{5.5}$$

where u_k are the exact eigenvectors; it is easy to show that

$$\gamma_k^{(i+1)} = \frac{\gamma_k^{(i)}}{\lambda_k - \lambda_g} \tag{5.6}$$

Thus the new vector is richer in the desired eigenvector than the guess, provided that the original guess is not pathologically deficient in this eigenvector ($\gamma_k^{(i)} = 0$).

The above technique is applicable to problems with Neumann or Dirichlet boundary conditions; periodicity requires special treatment since the matrix is cyclic. Since this does not arise in the annulus models it will not be considered here; however some methods are given by Temperton (1975).

The solution of the numerical analogue of equation (3.11) is performed using the standard algorithm described in FP I § 5.1. This again is not applicable to periodic problems.

6. APPLICATION TO SYMMETRIC GRIDS

It is clear that if the problem has degenerate eigenvalues, the methods of § 5 for the determination of eigenvectors will run into difficulties. It may be anticipated that periodic boundary conditions may yield degeneracies since the grid will support both sine and cosine functions. In practice it is also found that the most negative eigenvalues of a symmetric system also become pathologically close. It is mandatory to eliminate this problem by taking advantage of the symmetry; furthermore this is computationally beneficial by reducing the size of the vectors to be stored and the number of operations in the transforms of equations (3.2).

The presence of symmetry implies that the magnitude of an eigenvector should be the same at corresponding points, and that all pairs must be of the same sign or all of opposite sign. Therefore the vectors split into two sets, since an "even" vector is orthogonal to an "odd" vector. The number of vectors in each set is $\frac{I-2}{2}$. By setting the two central values to be either equal or of opposite sign, alternative boundary conditions may be generated for two matrices of half the size of the original,

which may then be solved as above. (This assumes an even number of gridpoints; a similar analysis may be performed if this number is odd.) If corresponding points in the function S of equation (3.1) are denoted S_a and S_b, then two vectors of length $\frac{I-2}{2}$ may be generated by taking combinations $\frac{1}{2}(S_a + S_b)$ and $\frac{1}{2}(S_a - S_b)$; the first vector is transformed using the even eigenvectors and the second with the odd eigenvectors. The two sets of equations (3.11) are completely independent.

Taking account of symmetry in this way means that a symmetrically stretched periodic grid may be employed using only the methods described, since the two "half-grids" are open-ended.

7. COMPARISON OF METHODS FOR SOLUTION OF POISSON'S EQUATION

This comparison of the ADI and direct method of solution will be made with respect to a two-dimensional non-uniform grid, with the number of gridpoints i by k, and assuming that the grid in the second direction is symmetric such that the second $k/2$ points are a reflection of the first $k/2$ points about the central point. Specifically a typical grid with 16 x 16 points will be considered, and 8 ADI iterations assumed since experience indicates that this is the minimum number required to maintain stability. The numbers of additions plus subtractions, and multiplications plus divisions, are evaluated by neglecting the "end effects" due to applications of boundary conditions, a procedure which will give a good approximation for large grids. The results may be found in Tables 1 and 2. It may be seen that the direct solution requires only c.30% of the operations needed for an ADI solution. In practice it is found that the overall execution time for the two-dimensional model, of which solution of Poisson's equation is only a part, is reduced by 22%.

If the formulae for a square mesh are equated, and terms in n neglected, a break-even point is obtained at about n = 65 (depending on the relation speeds of addition and multiplication). Thus up to this point the direct solution is not only more accurate but is also faster than the ADI technique.

Table 1 Operations for ADI

	+ −	x ÷
Rectangular mesh, per cycle	$10ik + 3(i + k)$	$12ik + 2(i + k)$
Square mesh, per cycle	$10n^2 + 6n$	$12n^2 + 4n$
16 x 16 mesh, per cycle	2656	3136
16 x 16 mesh, 8 cycles	21248	25088

Table 2 Operations for direct solution

	+ −	x ÷
Rectangular mesh	$\frac{5}{4}ik^2 + \frac{11}{2}ik + i$	$\frac{5}{4}ik^2 + \frac{13}{2}ik + i$
Square mesh	$\frac{5}{4}n^3 + \frac{11}{2}n^2 + n$	$\frac{5}{4}n^3 + \frac{13}{2}n^2 + n$
16 x 16 mesh	6544	6800

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